DETECTION OF INTERSTELLAR ETHYL CYANIDE

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ABSTRACT

Twenty-four millimeter-wave emission lines of ethyl cyanide (CH_3CH_2CN) have been detected in the Orion Nebula (OMC-1) and seven in Sgr B2. To derive precise radial velocities from the astronomical data, the first laboratory measurement of the rotational spectrum of ethyl cyanide has been made at frequencies above 41 GHz. In OMC-1, the rotational temperature of ethyl cyanide is 90 K (in good agreement with other molecules), the local standard of rest radial velocity is 4.5 ± 1.0 km s^{-1} (versus 8.5 km s^{-1} for most molecules), and the column density is 1.8×10^{14} cm^{-2} (a surprisingly high figure for a complicated molecule). The high abundance of ethyl cyanide in the Orion Nebula suggests that ethane and perhaps larger saturated hydrocarbons may be common constituents of molecular clouds and have escaped detection only because they are nonpolar, or only weakly so.

Subject headings: interstellar: abundances — interstellar: molecules — nebulae: Orion Nebula — radio sources: lines

I. INTRODUCTION

Cyanide compounds have been found to be quite abundant and to occur in great variety in the interstellar medium. During the past few years CN (Jefferts, Penzias, and Wilson 1970), HCN (Snyder and Buhl 1971), C_3N (Guelin and Thaddeus 1977), HC_3N (Turner 1971), HC_5N (Avery *et al.* 1976), CH_3CN (Solomon *et al.* 1971), and CH_2CHCN (Gardner and Winnewisser 1975) have all been detected in interstellar sources. We now report the detection of an even larger (nine atoms) and spectroscopically more complex cyanide compound, ethyl cyanide (CH_3CH_2CN). The 24 ethyl cyanide transitions observed thus far in Orion allow for determination of both the rotational partition function and the total column density. In addition, the spectrum observed toward Orion is centered at a local standard of rest (LSR) velocity of 4.5 km s^{-1} which is significantly lower than the velocity at which the main features of other molecules are found.

II. LABORATORY SPECTRUM

The microwave spectrum of ethyl cyanide was first studied in the laboratory by R. G. Lerner and B. P. Dailey in 1957. They concluded that, although the CH_3 group was free to rotate about the C—C bond, the potential barrier to this internal motion was quite

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large and at least the first few rotational transitions in the ground vibrational state could be treated as if the molecule were rigid. Laurie (1959), and later Mader, Heise, and Dreizler (1973) and Heise, Lutz, and Dreizler (1974) all reported detailed analyses of the ethyl cyanide spectrum in the 17–41 GHz region, confirming the high barrier to internal motion and the resulting lack of splittings in observed transitions. These efforts have resulted in an accurate structure for ethyl cyanide as well as a careful determination of the ^{14}N quadrupole coupling tensor. Heise, Lutz, and Dreizler also report the components of the permanent electric dipole moment along the two principal axes to be $\mu_a = 3.84(1)$ debye and $\mu_b = 1.37(1)$ debye.

All of these previous studies were limited to frequencies below 41 GHz and rotational quantum numbers below $J = 7$. Predictions of the millimeter-wave (80–120 GHz) spectrum of ethyl cyanide from these data with an accuracy of ~20 parts per million (ppm) were insufficient for astronomical purposes. We have therefore reinvestigated the laboratory spectrum of ethyl cyanide and obtained the new set of millimeter-wave measurements reported in Table 1. This new set of ethyl cyanide measurements has been combined with all of the data from the previously cited references in a simultaneous least-squares fit to the molecular Hamiltonian of Watson (1967) by using the techniques of Kirchhoff (1972). The rotational parameters resulting from this fit and their statistical errors are given in Table 2. These parameters were also used

TABLE 1

MILLIMETER-WAVELENGTH LABORATORY MEASUREMENTS OF ROTATIONAL
TRANSITIONS OF ETHYL CYANIDE (C_2H_5CN)

Measured Frequency (MHz)	Transition $J'_{K'_-,K'_+} - J''_{K''_-,K''_+}$	$\Delta\nu$ (obs.-calc.) (MHz)	Calc. Uncertainty (MHz)
89 627.98±0.17	$10_{3,8} - 9_{3,7}$	−0.43	0.07
89 684.76±0.17	$10_{3,7} - 9_{3,6}$	0.09	0.07
90 453.26±0.17	$10_{2,8} - 9_{2,7}$	−0.07	0.07
91 549.18±0.13	$10_{1,9} - 9_{1,8}$	0.08	0.07
98 532.26±0.10	$\begin{cases} 11_{8,3} - 10_{8,2} \\ 11_{8,4} - 10_{8,3} \end{cases}$	0.25	0.11
98 534.02±0.10	$\begin{cases} 11_{5,7} - 10_{5,6} \\ 11_{5,6} - 10_{5,5} \end{cases}$	0.10	0.06
98 544.23±0.10	$\begin{cases} 11_{9,2} - 10_{9,1} \\ 11_{9,3} - 10_{9,2} \end{cases}$	0.11	0.15
98 559.73±0.10	$\begin{cases} 11_{10,1} - 10_{10,0} \\ 11_{10,2} - 10_{10,1} \end{cases}$	−0.18	0.19
98 564.94±0.20	$11_{4,8} - 10_{4,7}$	0.16	0.06
98 566.28±0.20	$11_{4,7} - 10_{4,6}$	−0.46	0.06
98 610.25±0.19	$11_{3,9} - 10_{3,8}$	0.19	0.06
98 701.07±0.19	$11_{3,8} - 10_{3,7}$	0.01	0.06
103 867.74±0.11	$21_{1,20} - 21_{0,21}$	0.02	0.27
104 105.82±0.19	$13_{0,13} - 12_{1,12}$	0.13	0.08
104 359.66±0.11	$16_{3,13} - 16_{2,14}$	0.01	0.18
111 943.85±0.18	$18_{2,17} - 18_{1,18}$	−0.03	0.26
112 521.72±0.09	$11_{3,8} - 11_{2,9}$	−0.08	0.14
112 646.35±0.09	$13_{1,13} - 12_{1,12}$	0.16	0.09
113 502.34±0.09	$10_{3,7} - 10_{2,8}$	0.12	0.14
113 913.39±0.09	$14_{0,14} - 13_{1,13}$	0.08	0.11
113 978.03±0.13	$13_{0,13} - 12_{0,12}$	−0.18	0.09
114 188.45±0.09	$17_{1,16} - 16_{2,15}$	−0.04	0.23
115 894.18±0.20	$13_{2,12} - 12_{2,11}$	−0.17	0.09
116 578.99±0.27	$13_{3,11} - 12_{3,10}$	−0.24	0.08
116 788.71±0.20	$13_{3,10} - 12_{3,9}$	0.10	0.07
118 594.25±0.10	$13_{3,11} - 13_{2,12}$	−0.05	0.21
118 653.26±0.13	$13_{1,12} - 12_{1,11}$	0.22	0.08

during the fitting process to generate the predicted spectrum, which produced the $\Delta\nu$ values, for comparison, in column (3) and the associated standard deviations in column (4) of Table 1. It can be seen from Table 1 that, at the quoted 90% confidence level (2 times the standard deviation of the predicted frequency), the millimeter-wave spectrum can now be predicted about as well as it can be measured in the laboratory (~1 ppm). Accuracy in the measurements is limited by the broad lines observed in the laboratory (greater than or equal to 0.5 MHz) which are due to the combined effects of the large dipole moment (pressure broadening) and unresolved splittings from ^{14}N quadrupole (~0.1 MHz) and internal rotation.

III. OBSERVATIONS AND IDENTIFICATION

The observations reported here were obtained at the 11 m (36 foot) radio telescope of the National Radio Astronomy Observatory.[1] While pursuing other molecular observations during 1975 and early 1976, the

TABLE 2

DETERMINABLE ROTATIONAL PARAMETERS
FOR ETHYL CYANIDE

Parameter	Value (MHz)
A''	27663.661 (36)
B''	4714.1441 (43)
C''	4235.0412 (40)
τ_1	0.15323 (26)
τ_2	0.01169 (7)
τ_3	1.111 (8)
τ_{aaaa}	-1.995 (12)
τ_{bbbb}	-0.017751 (50)
τ_{cccc}	-0.0067873 (452)
Standard deviation...	0.14

Harvard observers detected a number of emission lines of unknown molecular origin in the frequency range of 98–116 GHz. These observations were communicated to the National Bureau of Standards, where ethyl cyanide was identified as the molecular source of these lines. Independently, in 1976 April, the Goddard observers detected a number of emission features between 88 and 100 GHz, which they identified as rotational line emission from ethyl cyanide. The present paper is the result of combining these independent astronomical and laboratory measurements on the ethyl cyanide molecule.

a) Orion A

All observations reported for Ori A were obtained toward the Kleinmann-Low region [α(1950) = $5^h32^m47^s$; δ(1950) = $-5°24'21''$]. Owing to the low intensity of the observed lines, no attempt was made to map this cloud. Table 3 summarizes the emission lines which we have observed thus far in this source. The identification of ethyl cyanide as the molecular source was convincingly established from (*a*) the systematic correlation between the calculated laboratory rest frequencies shown in column (1) of Table 3 and the rest frequencies derived from the Ori A observations, and (*b*) the excellent agreement between
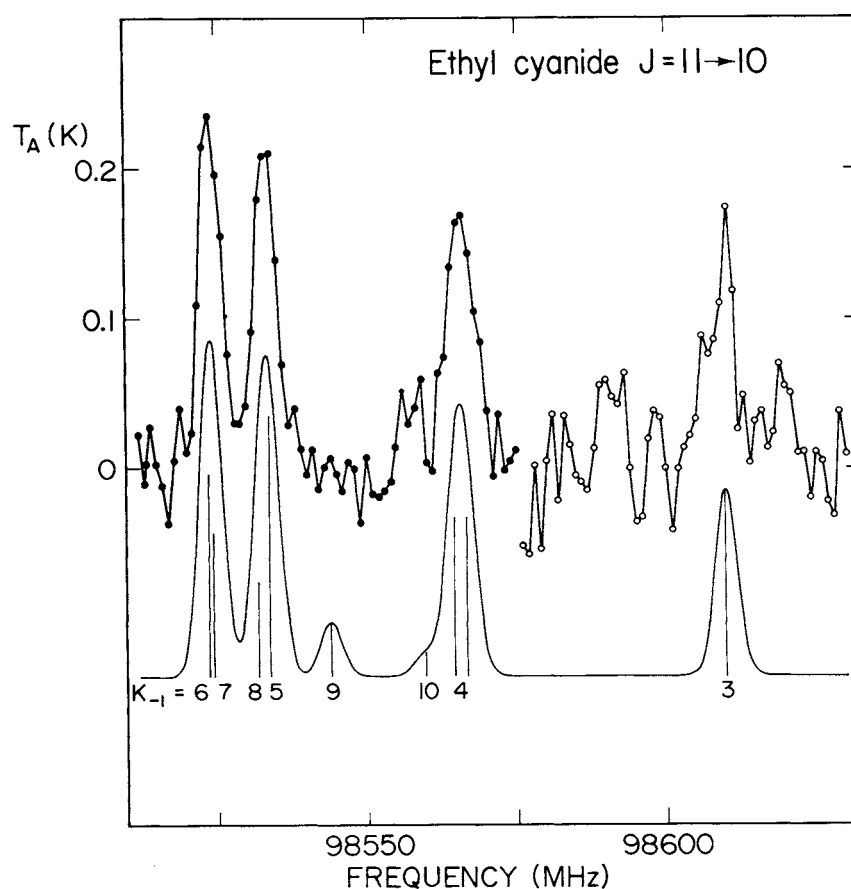

FIG. 1.—A portion of the ethyl cyanide $J = 11 \rightarrow 10$ transitions observed toward Ori A. The upper curve shows the observed spectrum; the lower curve is the theoretical spectrum computed assuming low optical depth, thermodynamic equilibrium with a temperature of 90 K, and a beam-averaged column density of 1.8×10^{14} cm^{-2}. The resolution is 1 MHz. The figure is composed from two sets of data taken at slightly different local oscillator settings. The lower-frequency section (*filled circles*) had approximately twice the integration time used for the higher-frequency section (*open circles*). The intensity of the higher-frequency section was adjusted by 5% so that the $K = 4$ line observed in both settings agreed.

TABLE 3

INTERSTELLAR ETHYL CYANIDE EMISSION LINES OBSERVED TOWARD ORION A

Calculated Rest Frequency (MHz)	Transition $J'_{K'_-,K'_+} - J''_{K''_-,K''_+}$	T_A^* (K) (obs.)	T_A (K)[†](calc.)	Δν(obs.-calc) with $V_{LSR}=4.5$ km s^{-1} (MHz)
88 323.72(8)	$10_{0,10} - 9_{0,9}$	0.12±0.05	0.13	1.1±1.4
89 562.24(7)	$10_6 - 9_6$	0.08‡	0.11	-0.2±0.05
89 564.95(8)	$10_7 - 9_7$	0.05‡	0.07	
89 568.03(6)	$10_5 - 9_5$	0.11‡	0.14	
89 572.98(11)	$10_8 - 9_8$	0.03‡	0.04	
89 589.98(6)	$10_{4,7} - 9_{4,6}$	0.05‡	0.09	0.1±0.6
89 590.96(6)	$10_{4,6} - 9_{4,5}$	0.05‡	0.09	
89 628.41(7)	$10_{3,8} - 9_{3,7}$	0.13±0.05	0.11	0.1±0.5
95 442.44(8)	$11_{1,11} - 10_{1,10}$	0.20±0.07	0.14	-1.2±1.7
96 919.71(8)	$11_{0,11} - 10_{0,10}$	0.08±0.03	0.15	-0.2±1
98 177.55(7)	$11_{2,10} - 10_{2,9}$	0.15±0.05	0.14	-0.8±0.7
98 523.80(7)	$11_6 - 10_6$	0.13±0.01‡	0.13	0.0±0.1
98 524.58(9)	$11_7 - 10_7$	0.10±0.01‡	0.10	
98 532.01(12)	$11_8 - 10_8$	0.06±0.01‡	0.06	0.0±0.15
98 533.91(6)	$11_5 - 10_5$	0.17±0.01‡	0.17	
98 564.78(6)	$11_{4,8} - 10_{4,7}$	0.09±0.01‡	0.11	0.1±0.25
98 566.74(6)	$11_{4,7} - 10_{4,6}$	0.09±0.01‡	0.11	
98 610.07(6)	$11_{3,9} - 10_{3,8}$	0.14±0.03	0.12	-0.6±0.6
98 701.07(6)	$11_{3,8} - 10_{3,7}$	0.12±0.05	0.12	0.2±1
100 614.28(7)	$11_{1,10} - 10_{1,9}$	0.10±0.03	0.15	-0.5±0.5
104 051.24(8)	$12_{1,12} - 11_{1,11}$	0.08±0.06	0.16	+1.0±1
109 650.29(6)	$12_{1,11} - 11_{1,10}$	0.07±0.05	0.17	-2±1
113 978.21(10)	$13_{0,13} - 12_{0,12}$	0.12±0.05	0.18	-0.5±1
115 894.35(9)	$13_{2,12} - 12_{2,11}$	0.09±0.05	0.17	-2±1

[†] The calculated intensities are for T = 90 K and a total column density NL = 1.8×10^{14} cm^{-2}, under the assumption of low optical depth and thermodynamic equilibrium with ΔV = 12.5 km s^{-1}.

‡ These lines are blended. The observed intensities were obtained from the best theoretical fit to the observed profiles assuming a 12.5 km s^{-1} line width. See Figures 1 and 2.

the observed and calculated relative intensities illustrated in Figures 1 and 2.

Column (3) of Table 3 lists the brightness temperature, T_A^*, for the lines observed in Ori A. It should be noted that these observations were made over an extended period of time and that the majority of them were obtained with a double-sideband observing mode. The best velocity determination was obtained from the quartet pattern of the $J = 11 \rightarrow 10$ K doublets shown in Figure 1. These features were least-squares fitted to a theoretical spectrum with V_{LSR}, ΔV, T_{kin}, and NL (the column density) as variables. Since a number of the observed features are a blend of several lines, these were fitted with a function formed by the sum of several Gaussians of identical width; each Gaussian represented a single transition, and the rest frequency was fixed at the values shown in column (1)

of Table 3. The theoretical relative intensity for the transitions was computed assuming low optical depth and thermodynamic equilibrium. The observed and theoretical spectra are shown in Figure 1. The results of this fit are $V_{LSR} = +4.5 \pm 1$ km s^{-1}, $\Delta V = 12.5 \pm 1$ km s^{-1}, $T_{kin} = 90$ K, and a beam-averaged total column density of 1.8×10^{14} cm^{-2}. While a kinetic temperature of 90 K provides the best fit to the observations, the observations are consistent with a range of temperature of 50–200 K. Thus the column density ranges from 1.3×10^{14} cm^{-2} for $T_{kin} = 50$ K to 3.9×10^{14} cm^{-2} for $T_{kin} = 200$ K, with 1.8×10^{14} cm^{-2} the most probable value.

Since the $J = 10 \rightarrow 9$ spectral lines near 89.5 GHz are more severely blended, the theoretical spectrum, shown below the observed spectrum in Figure 2, was calculated with T_{kin}, V_{LSR}, and ΔV fixed at the values
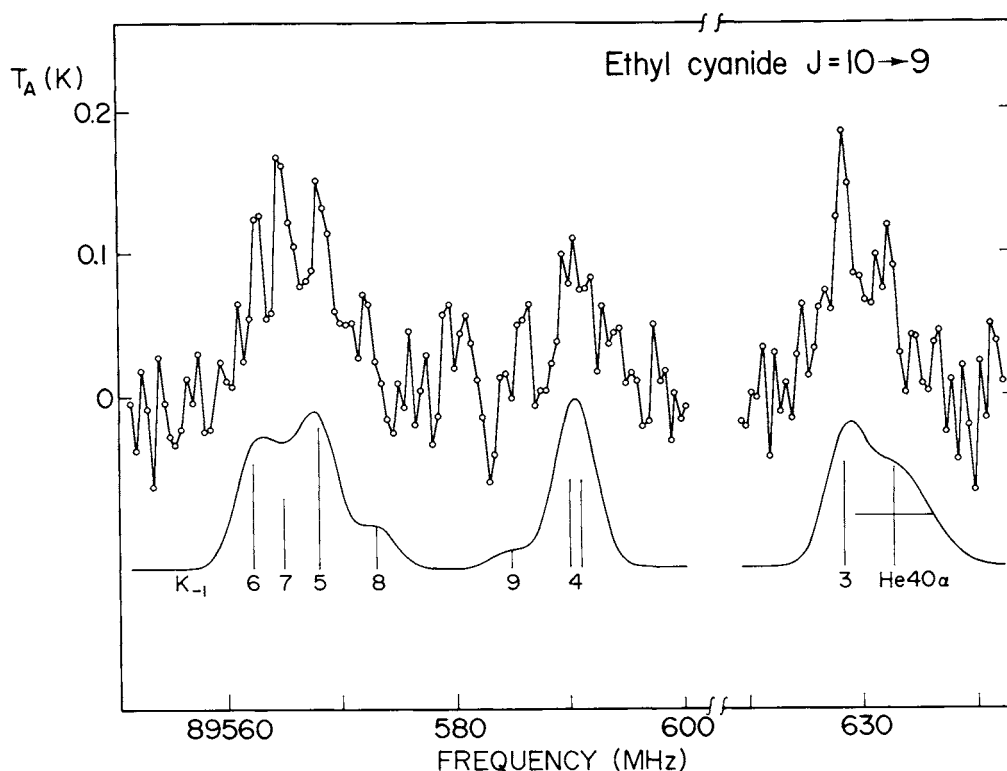
FIG. 2.—A portion of the $J = 10 \to 9$ ethyl cyanide lines observed toward Ori A with 0.5 MHz resolution is shown in the upper tracing. The theoretical spectrum, shown in the lower part of the figure, was computed with a beam-averaged column density of 1.4×10^{14} cm^{-2}. The $K_{-1} = 3$ line is blended with the He 40α line (99,063.3 MHz) which falls in the upper sideband of the receiver.

obtained for the $J = 11 \to 10$ fit. Good agreement was obtained between the observed and calculated intensities with a column density of 1.4×10^{14} cm^{-2}.

Column (3) of Table 3 shows the observed intensities for all of the ethyl cyanide lines detected in Ori A. For comparison, theoretical intensities obtained with $\Delta V = 12.5$ km s^{-1}, $T = 90$ K, and $NL = 1.8 \times 10^{14}$ cm^{-2} are given in column (4) of Table 3. The last column of this table shows the deviations obtained between the Ori A observations with $V_{\mathrm{LSR}} = +4.5$ km s^{-1} and the calculated laboratory rest frequencies given in column (1). The overall agreement within the quoted uncertainties is very satisfying.

b) *Sagittarius B2*

Ethyl cyanide was also detected in very weak emission from the direction of Sgr B2 [α(1950) = $17^{\mathrm{h}}44^{\mathrm{m}}11^{\mathrm{s}}$; δ(1950) = $-28°22'30''$], as indicated in Table 4. On the average, the signals from Sgr B2 are a factor of 2 less intense than those from Orion and generally in agreement with the usual velocity of 62 km s^{-1} and width of 18 km s^{-1}. Assuming local thermodynamic equilibrium with $T = 20$ K and low optical depth, we determine a total column density of 0.9×10^{14} cm^{-2} for ethyl cyanide in Sgr B2. If the kinetic temperature were higher, say, 60 K, the column density for ethyl cyanide would be 1.6×10^{14} cm^{-2}.

c) *Other Regions*

Ethyl cyanide was searched for unsuccessfully in several other interstellar sources. The 11_4–10_4 K doublet near 98.5 GHz was not detected in IRC $+10216$ at a level less than 0.04 K or in DR 21 at a level less than 0.06 K.

d) *Vinyl Cyanide*

We have observed an emission line at 94,277 MHz (assuming $V_{\mathrm{LSR}} = 62$ km s^{-1}) in Sgr B2. This line

TABLE 4
EYTHL CYANIDE EMISSION LINES OBSERVED TOWARD SAGITTARIUS B2

Calculated Rest Frequency*	Transition	T_A* (K)
91549.10 (7)	$10_{1,9}$–$9_{1,8}$	0.20 ± 0.05
95442.44 (8)	$11_{1,11}$–$10_{1,10}$	0.14 ± 0.06
96919.71 (8)	$11_{0,11}$–$10_{0,10}$	0.05 ± 0.02
98564.78 (6)	$11_{4,8}$–$10_{4,7}$	$\left.\right\}$ 0.05 ± 0.02
98566.74 (6)	$11_{4,7}$–$10_{4,6}$	
98610.07 (6)	$11_{3,9}$–$10_{3,8}$	0.08 ± 0.04
98701.07 (6)	$11_{3,8}$–$10_{3,7}$	0.08 ± 0.04

* All lines were consistent with $V_{\mathrm{LSR}} \approx 62$ km s^{-1} and an average width of $\Delta V \approx 18$ km s^{-1}.

coincides with the $10_{0,10}$–$9_{0,9}$ transition of vinyl cyanide (CH_2CHCN), with a calculated rest frequency of $94,276.6 \pm 0.4$ MHz. The observed brightness temperature is 0.08 ± 0.03 K, with a width $\Delta V = 16.7$ km s^{-1}. Assuming LTE with a kinetic temperature of 20 K, the column density of CH_2CHCN derived from this observation is 3×10^{13} cm^{-2}.

Vinyl cyanide was not detected toward Ori A. An upper limit of 0.13 K was obtained for the $10_{0,10}$–$9_{0,9}$ and $11_{1,11}$–$10_{1,10}$ transitions in Ori A. Assuming LTE with $T = 90$ K and $\Delta V = 15$ km s^{-1}, a conservative upper limit derived for the vinyl cyanide column density is less than 1.5×10^{14} cm^{-2}.

IV. DISCUSSION

Ethyl cyanide has been firmly established as an important constituent of the molecular clouds associated with Orion and Sgr B2. The large number of observed signals obtained for ethyl cyanide allows the determination of the total column density with higher confidence than is typically possible for weak lines. The total column density for ethyl cyanide was found to be 1.8 ($+2.1$, -0.5) $\times 10^{14}$ cm^{-2} in Orion and 0.9×10^{14} cm^{-2} in Sgr B2.

Ethyl cyanide appears to exist in a region of the Orion Molecular Cloud characterized by $V_{LSR} = 4.5 \pm 1$ km s^{-1} and $\Delta V \approx 12.5$ km s^{-1}. It should be noted that the 21 cm hydrogen line, which is generally thought to originate in a low-density region in front of the Orion Molecular Cloud, also occurs at a velocity $V_{LSR} \approx 5$ km s^{-1}. Broad features in Orion are somewhat unusual, although several molecules show emission which is characterized by a spike feature centered at 8.5 km s^{-1} with $\Delta V \approx 4.5$ km s^{-1} and a plateau feature centered at a slightly higher velocity with $\Delta V \approx 30$ km s^{-1}. A recent observation of SO_2 (Snyder et al. 1975) clearly illustrates these two features in a single Orion spectrum and shows an additional shoulder or spike centered at $V_{LSR} \approx +3$ km s^{-1}. A recent report by Barrett, Ho, and Meyers (1977) on NH_3 in Orion presents probably the best case for the existence of this low-velocity feature, again as a shoulder on a dominant feature centered roughly at 8 km s^{-1}. Many additional unidentified interstellar lines are known to exist in Orion which seem to be characterized by the width $\Delta V \approx 12$–15 km s^{-1}. It will be interesting to see if these lines can be assigned to other big molecules of complex chemical origin with $V_{LSR} \approx 4.5$ km s^{-1}.

By way of comparison, the column densities of ethyl cyanide, vinyl cyanide, cyanoacetylene, and methyl cyanide are given in Table 5. Quite surprisingly, in Orion the ethyl cyanide, and possibly the vinyl cyanide, column densities are about 5 times larger than that of the simpler cyanoacetylene. However, in Sgr B2 the column densities are more nearly equal, but that of cyanoacetylene is the largest.

TABLE 5

COLUMN DENSITIES FOR SEVERAL LARGE CYANIDE COMPOUNDS IN ORION A AND SAGITTARIUS B2

MOLECULE	COLUMN DENSITY (10^{14} cm^{-2}) Orion A	Sagittarius B2	REFERENCE
CH_3CH_2CN	1.8	0.9	Present paper
CH_2CHCN	< 1.5	0.3	Present paper
HCCCN	0.24	2.0	Morris et al. 1976*
CH_3CN	1	1	Present paper†

* For Ori A a kinetic temperature of 50 K was assumed, and 25–50 K for Sgr B2.

† The Ori A value was determined from the $J = 5$–4 lines reported by Lovas et al. 1976 with $T_{kin} = 90$ K. The Sgr B2 density was determined from the $J = 6_0$–5_0 observations of Solomon et al. 1971 with $T_{kin} = 50$ K.

These comparisons suggest that, at least in Orion, hydrogen-saturated compounds like ethyl cyanide are highly favored. It follows that symmetric hydrogen-saturated compounds, such as ethane (C_2H_6), could indeed be very abundant. Unfortunately, symmetric paraffins like ethane cannot be observed by radio techniques since they are nonpolar. The CN radical is an excellent symmetry-breaking tag for these compounds, since the resulting cyanide molecules have large dipole moments and characteristically intense spectra. Saturated asymmetric hydrocarbons, such as propane, tend to have small dipole moments and would therefore remain undetectable even at fairly substantial concentrations. However, alkane derivatives containing the CN, OH, or NH_2 groups are quite polar and are more readily detectable in interstellar clouds. Since two of the ethane derivatives, ethyl alcohol and ethyl cyanide, have already been detected in Sgr B2, we expect that ethylamine would also be observable, as should some of the analogous propane derivatives, particularly when they exhibit a pileup of a-type R-branch transitions similar to that in the ethyl cyanide spectrum.

The large number of transitions reported here for ethyl cyanide clearly indicates the future usefulness of molecules of this size as astrophysical probes for characterizing molecular clouds and interstellar chemistry. The growing list of interstellar cyanide compounds which may be chemically related, e.g., C_3N, HC_3N, CH_2CHCN, and CH_3CH_2CN, suggests more detailed studies of their emission lines—first, to determine if they coexist in the same molecular cloud, and second, to obtain more accurate densities as a basis for modeling the chemical formation process.

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